

Quantifying Quantum Correlations in Fermionic Systems using Witness Operators

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(Dated: February 22, 2013)

We present a method to quantify quantum correlations in arbitrary systems of indistinguishable fermions using witness operators. The method associates the problem of finding the optimal entanglement witness of a state with a class of problems known as semidefinite programs (SDPs), which can be solved efficiently with arbitrary accuracy. Based on these optimal witnesses, we introduce a measure of quantum correlations which has an interpretation analogous to the Generalized Robustness of entanglement. We also extend the notion of quantum discord to the case of indistinguishable fermions, and propose a geometric quantifier, which is compared to our entanglement measure. Our numerical results show a remarkable equivalence between the proposed Generalized Robustness and the Schliemann concurrence, which are equal for pure states. For mixed states, the Schliemann concurrence presents itself as an upper bound for the Generalized Robustness. The quantum discord is also found to be an upper bound for the entanglement.

PACS numbers: 03.67.-a

I. INTRODUCTION

The notion of entanglement, first noted by Einstein, Podolsky and Rosen [1], is considered one of the main features of quantum mechanics, being subject of study in several areas recently [2–4]. Thus, it is of paramount importance both the understanding and the quantification of entanglement in composite quantum systems, being these one of the main challenges of modern quantum theory.

Despite being a subject widely studied in systems of non-identical particles, or whose particles, though identical, are well separated from each other, being thus distinguishable, less attention was given to the case where this separation is very small, such that the overlap of their wave functions is no longer negligible. In this case we have to take into account the indistinguishability of the particles, being the space of quantum states restricted to symmetric or antisymmetric subspaces of the Hilbert space, depending on the bosonic or fermionic nature of the system. The study of entanglement for systems of indistinguishable particles has been, however, a subject of great controversy, leading to different approaches in its treatment. Among the most mentioned we have: quantum correlations [5], entanglement of modes [6], entanglement of particles [7]. The concept of quantum correlations is based on the notion that the correlations generated by mere (anti-)symmetrization of the state due to indistinguishability of their particles do not constitute truly as entanglement. We will analyse, in this paper, the quantum correlations in systems of indistinguishable

fermions.

The entanglement in two-fermion states with a four-dimensional single-particle space ($\mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$) can be characterized by the Schliemann concurrence [5]. For pure states in arbitrary dimension, one can use the von Neumann entropy of the reduced single-particle density matrix as a measure of entanglement [8]. However, the problem of quantification or even detection of entanglement in the general case is still open [9–11]. A useful concept is that of entanglement witness [12]: a Hermitian operator with non-negative expectation value for all separable states, but which can have a negative expectation value for an entangled state. We will focus on optimal entanglement witnesses (OEWS), that can be used not only to *witness* the entanglement, but also to quantify it [13–15]. In this paper, we will see how to determine such OEWS, and especially how to use them to quantify the quantum correlations in fermionic systems. We will also confront our measure of entanglement with the *quantum discord* [16–19]. In order to do that, we will define a quantum discord for fermionic particles. Previous studies of quantum discord in systems of indistinguishable particles, like in [20], employ the notion of correlation of modes [6], which are distinguishable.

This paper is organized as follows. In Sec.II we recall some known concepts and tools of the theory of entanglement, as the witnessed entanglement and the quantum correlations, which will be essential to the development of the ideas throughout the article. In Subsec.II A, we recall the definition of optimal entanglement witness, and briefly discuss its use as an entanglement quantifier. In Subsec.II B we recall the ideas associated with the concept of quantum correlations, as well as the Schliemann concurrence. In Subsec.II C we revise the concept of quantum discord for distinguishable particles. In Sec.III we introduce our method for quantifying the quantum correlations in fermionic systems using witness operators, and define the Fermionic Generalized Robust-

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ness. We also extend the notion of quantum discord to fermions, such that it takes into account the particles' indistinguishability, and introduce the *Fermionic Geometric Discord*. In Sec.IV we show numerical results, comparing the Fermionic Generalized Robustness, the Schliemann concurrence, and the Fermionic Geometric Discord. We finish the illustration of the method with a beautiful *quantum phase diagram* yielded by the five-partite Fermionic Generalized Robustness in the Extended Hubbard Model. We conclude in Sec.V.

II. PRELIMINARY CONCEPTS

We will see, in this section, some familiar concepts from the theory of entanglement, namely, *witnessed entanglement* [13–15], quantum correlations [5] and quantum discord [16–19]. A reader already familiarized with such concepts might skip to the next section of the article.

A. Witnessed Entanglement

Entanglement witnesses are Hermitian operators (observables - W) whose expectation values contain information about the entanglement of quantum states. The operator W is an entanglement witness for a given entangled quantum state ρ if the following conditions are satisfied [12]: its expectation value is negative for the particular entangled quantum state ($\text{Tr}(W\rho) < 0$), while it is non-negative on the set of separable states (S) ($\forall \sigma \in S, \text{Tr}(W\sigma) \geq 0$). We are particularly interested in optimal entanglement witnesses. W_{opt} is the OEW for the state ρ if

$$\text{Tr}(W_{opt}\rho) = \min_{W \in \mathcal{M}} \text{Tr}(W\rho), \quad (1)$$

where \mathcal{M} represents a compact subset of the set of entanglement witnesses \mathcal{W} .

OEWs can be used to quantify entanglement. Such quantification is related to the choice of the set \mathcal{M} , where different sets will determine different quantifiers [13]. We can define these quantifiers by:

$$E(\rho) = \max(0, -\min_{W \in \mathcal{M}} \text{Tr}(W\rho)). \quad (2)$$

An example of a quantifier that can be calculated using OEW is the Generalized Robustness of entanglement [22] ($\mathcal{R}_g(\rho)$), which is defined as the minimum required mixture such that a separable state is obtained. Precisely, it is the minimum value of s such that

$$\sigma = \frac{\rho + s\varphi}{1 + s} \quad (3)$$

be a separable state, where φ can be any state. We know that the Generalized Robustness can be calculated from

Eq.2, using $\mathcal{M} = \{W \in \mathcal{W} | W \leq I\}$ [13], where I is the identity operator; in other words,

$$\mathcal{R}_g(\rho) = \max(0, -\min_{\{W \in \mathcal{W} | W \leq I\}} \text{Tr}(W\rho)). \quad (4)$$

The construction of entanglement witnesses is a hard problem. In an interesting method proposed by Brandão and Vianna [14], the optimization of entanglement witnesses is cast as a *robust semidefinite program* (RSDP). Despite RSDP is computationally intractable, it is possible to perform a probabilistic relaxation turning it into a semidefinite program (SDP), which can be solved efficiently [23].

B. Quantum Correlations

The space state for indistinguishable fermions is antisymmetric under permutation of particles. In this case, it is convenient to use the *second quantization* formalism, in order to deal with the antisymmetric states in the *Fock space*. Accordingly we introduce an algebra of operators which satisfy the following anti-commutation relations:

$$\{f_i^\dagger, f_j^\dagger\} = \{f_i, f_j\} = 0, \quad \{f_i, f_j^\dagger\} = \delta_{ij}, \quad (5)$$

where f_i^\dagger and f_i are the fermionic creation and annihilation operators, respectively, so that their application on the vacuum state ($|0\rangle$) creates/annihilates a fermion in state “ i ”. The vacuum state is defined so that $f_i|0\rangle = 0$.

An immediate and disturbing consequence of the antisymmetric structure of the state space can be seen even in the simplest example of a two-fermion system, which, if analysed in the usual way, will always be considered entangled. We must therefore rethink the way entanglement is calculated for systems of indistinguishable particles, as well as its physical interpretation.

In the case which the identical particles are localized in *distinct* laboratories and *independently* prepared, it is natural to think that the entanglement calculated in the usual way should not have any relevant physical meaning; or rather, “no quantum prediction, referring to an atom located in our laboratory, is affected by the mere presence of similar atoms in remote parts of universe” [24].

We are interested in the case of identical particles that are sufficiently close together such that the overlap between their wave functions is no longer negligible, and therefore they are indistinguishable. Fermionic systems of this kind can be described using Slater determinants [4]. Consider, for example, a two-fermion state represented by a single Slater determinant, namely,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\phi\rangle \otimes |\chi\rangle - |\chi\rangle \otimes |\phi\rangle) = f_\phi^\dagger f_\chi^\dagger |0\rangle, \quad (6)$$

where $|\phi\rangle$ and $|\chi\rangle$ correspond to orthonormal wave functions (*spin-orbitals*). It is easy to see, in this simple case, that the anti-symmetrization of coordinates introduces correlations between the fermions, namely, the well

known *exchange contributions* from the Hartree-Fock theory. On the other hand, a single Slater determinant is solution of a one-particle Schrödinger equation and, therefore, can have no quantum correlation between the particles [4]. Considering states described by more than one Slater determinant introduces additional correlations beyond the exchange contribution. We will then interpret such additional correlations as the analog of quantum entanglement in systems of distinguishable particles, calling them as *fermionic entanglement* [5].

A measure of fermionic entanglement was proposed in [5] as the analogous of Wootters concurrence [25]. Notwithstanding, such measure, called Schliemann concurrence (C_S), is valid only for two-fermion states with a four-dimensional single-particle Hilbert space ($\mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$), i.e. the antisymmetric space of lowest dimension where can exist quantum correlated states.

In order to define the Schliemann concurrence, we have to introduce some operators. Let \mathcal{U}_{ph} be the operator of particle-hole transformation:

$$\mathcal{U}_{ph} f_i^\dagger \mathcal{U}_{ph}^\dagger = f_i, \quad \mathcal{U}_{ph} |0\rangle = \prod_{i=1}^d f_i^\dagger |0\rangle, \quad (7)$$

being d the single-particle Hilbert space dimension. Similarly, define \mathcal{K} as the anti-linear operator of complex-conjugation, satisfying the following relations:

$$\mathcal{K} f_i^\dagger \mathcal{K} = f_i^\dagger, \quad \mathcal{K} f_i \mathcal{K} = f_i, \quad \mathcal{K} |0\rangle = |0\rangle. \quad (8)$$

Thus, given the operator $\mathcal{D} = \mathcal{K} \mathcal{U}_{ph}$, called operator of dualisation, and the dual states $\tilde{\rho} = \mathcal{D} \rho \mathcal{D}^{-1}$, we have that the Schliemann concurrence for states $\rho \in \mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$ is given by

$$C_S(\rho) = \max(0, \lambda_6 - \lambda_5 - \lambda_4 - \lambda_3 - \lambda_2 - \lambda_1), \quad (9)$$

where λ_i 's are, in descending order of magnitude, the square roots of the singular values of the matrix $R = \rho \tilde{\rho}$.

C. Quantum Discord

The total amount of correlations (classical and quantum) carried in a bipartite system is quantified by the mutual information:

$$I(A : B) = S(A) + S(B) - S(A, B), \quad (10)$$

where $S(X)$ is the Shannon (von Neumann) entropy for the classical (quantum) system. In the classical case, the mutual information has another interpretation: it measures the decrease of ignorance about the subsystem A , when B is known. In this case, an equivalent expression for the mutual information reads:

$$J(A : B) = S(A) - S(A|B), \quad (11)$$

where

$$S(A|B) = \sum_b p_b S(A|b) \quad (12)$$

is the conditional entropy on A given B . In quantum systems this equivalence is not always true. The disagreement between these expressions is called *quantum discord*, and can be used to quantify quantum correlations [16]:

$$D(A : B) = I(A : B) - J(A : B). \quad (13)$$

However, there is an ambiguity in $J(A : B)$ due to the freedom of choice for the measurement operators, where for each set of measurements $\{\Pi_i\}_B$ on B , the conditional entropy value may be different and consequently also the mutual information. The quantum discord is thus redefined by minimizing its value over all measurement operators. The mutual information is thus properly defined by:

$$J(A : B) = S(A) - \max_{\{\Pi_i\}_B} S(A|B), \quad (14)$$

and it is known to quantify classical correlations [17]. Thus, the quantum discord measures the difference between the total and classical correlations on the system, therefore being a quantifier of quantum correlations. Note however that quantum discord is not a measure of entanglement, and quantum separable states usually have non-zero discord. The quantum states with null discord are those which are a mere encoding of classical statistical distributions, and can be written in the form:

$$\xi = \sum_{ij} \lambda_{ij} |e_i\rangle \langle e_i| \otimes |f_j\rangle \langle f_j|. \quad (15)$$

where $|e_i\rangle$ and $|f_j\rangle$ are orthonormal basis.

Given the set (Ω) of states with zero-discord, formed by the states above, it is clear that the minimal distance between a state ρ and this set can be used to quantify the quantum discord [18]:

$$\mathcal{D}(\rho) = \min_{\xi \in \Omega} |\xi - \rho|_p, \quad (16)$$

where $|A|_p$ is the Schatten p -norm. A usual measure of quantum discord is based on the 2-norm, or Hilbert-Schmidt norm, proposed by Dakić *et al.* [19].

III. QUANTIFYING QUANTUM CORRELATIONS USING WITNESS OPERATORS

In this section we will present our method for quantifying fermionic entanglement using witness operators. After defining the set of separable states pertinent to our case, i.e. the fermionic states without entanglement, we will introduce a method for determining OEWs. In particular, we will see which constraints to impose on the set \mathcal{M} of witnesses (Eq.2) in order to obtain a quantifier analogous to the Generalized Robustness (Eq.4). We also will define a notion of quantum discord for fermions and confront it to entanglement.

We know that states without entanglement are those that can be described by a single Slater determinant, or a convex mixture of them. Consider \mathcal{F}_n^d as the Fock space of n indistinguishable fermions sharing a d -dimensional single-particle Hilbert space. We have then the following definition of “separable” states:

State with no fermionic entanglement (separable): A state $\sigma \in \mathcal{B}(\mathcal{F}_n^d)$ has no fermionic entanglement if it can be decomposed as

$$\sigma = \sum_i p_i a_1^{i\dagger} \cdots a_n^{i\dagger} |0\rangle \langle 0| a_n^i \cdots a_1^i, \quad \sum_i p_i = 1, \quad (17)$$

where $a_k^{i\dagger} = \sum_{l=1}^d c_l^{ik} f_l^\dagger$, and $\{f_l^\dagger\}$ is an orthonormal basis of fermionic creation operators for the space of a single fermion (\mathcal{F}_1^d). Of course, the states defined by Eq.17 are not separable in the usual mathematical sense, meaning that they are product states or convex mixtures of it. But we will insist in referring to them as *separable*, for they are just anti-symmetrization of the usual distinguishable separable states. Entanglement, in the case of distinguishable particles, is defined in opposition to separability, i.e., an entangled state is that one which is not separable. We want to keep this notion.

It is interesting to note that, as in the case of distinguishable particles, the set of separable states is invariant under *local operations*, taking now into account that the local operations must be symmetric, due to the indistinguishability of the particles. Let Φ be a *local symmetric operation* (LSO), i.e., an operation that respects the Pauli exclusion principle and does not involve any interaction between particles. An LSO can be written as:

$$\Phi(\rho) = \sum_i (M_i \otimes M_i \otimes \cdots \otimes M_i) \rho (M_i^\dagger \otimes M_i^\dagger \otimes \cdots \otimes M_i^\dagger) \quad (18)$$

where M_i is a linear operator acting on the Hilbert space of a single particle. Given a fermionic separable pure state (i.e. a single Slater determinant) $|\psi_{sep}\rangle = \mathcal{A}(|e_1\rangle \otimes \cdots \otimes |e_n\rangle)$, where \mathcal{A} is the anti-symmetrization operator, $\{|e_i\rangle\}$ is an orthonormal basis, and noting that $[\Phi, \mathcal{A}] = 0$, we see that

$$\begin{aligned} (M_i \otimes \cdots \otimes M_i) |\psi_{sep}\rangle &= (M_i \otimes \cdots \otimes M_i) \mathcal{A} |e_1 \cdots e_n\rangle \\ &= \mathcal{A} (M_i \otimes \cdots \otimes M_i) |e_1 \cdots e_n\rangle \\ &= \mathcal{A} |(M_i e_1) \cdots (M_i e_n)\rangle \\ &= \mathcal{A} |e'_1 \cdots e'_n\rangle \\ &= |\psi'_{sep}\rangle \end{aligned} \quad (19)$$

and such result clearly extends to mixed states. Summarizing, given a separable state $\sigma \in \mathcal{S}$, we have that $\Phi_{LSO}(\sigma) \in \mathcal{S}$, indicating that in order to have quantum entanglement, the particles must interact by means of some global operation.

Now we adapt Brandão and Vianna’s [14] technique in order to obtain a new algorithm to determine OEWs for

indistinguishable fermions in the Fock space. The new method can be enunciated as follows.

Determination of OEW using RSDP: A fermionic state $\rho \in \mathcal{B}(\mathcal{F}_n^d)$ is entangled if and only if the optimal value of the following RSDP is negative:

minimize $Tr(W\rho)$ subject to

$$\left\{ \begin{array}{l} \sum_{i_{n-1}=1}^d \cdots \sum_{i_1=1}^d \sum_{j_1=1}^d \cdots \sum_{j_{n-1}=1}^d (c_{i_{n-1}}^{n-1*} \cdots c_{i_1}^{1*} c_{j_1}^1 \cdots c_{j_{n-1}}^{n-1} \times \\ \quad W_{i_{n-1} \cdots i_1 j_1 \cdots j_{n-1}}) \geq 0, \\ \forall c_i^k \in \mathcal{C}, \quad 1 \leq k \leq (n-1), \quad 1 \leq i \leq d, \\ \mathcal{A}W\mathcal{A}^\dagger = W, \\ W \leq \mathcal{A}, \end{array} \right. \quad (20)$$

where d is the dimension of the single particle Hilbert space, $\{f_l^\dagger\}$ is an orthonormal basis of fermionic creation operators, \mathcal{A} is the anti-symmetrization operator, and $W_{i_{n-1} \cdots i_1 j_1 \cdots j_{n-1}} = f_{i_{n-1}} \cdots f_{i_1} W f_{j_1}^\dagger \cdots f_{j_{n-1}}^\dagger \in \mathcal{B}(\mathcal{F}_1^d)$ is an operator acting on the space of one fermion. The notation $W \leq \mathcal{A}$ means that $(\mathcal{A} - W) \geq 0$ is a positive semidefinite operator. If ρ is entangled, the operator W that minimizes the problem corresponds to the OEW of ρ .

Proof: It is known that a state is entangled if and only if there exists a witness operator W such that $Tr(W\rho) < 0$ and $Tr(W\sigma) \geq 0$ for every separable state σ . Consider a general separable state as given by Eq.17. The semi-positivity condition $Tr(W\sigma) \geq 0$ is equivalent to:

$$\langle 0 | a_n a_{n-1} \cdots a_1 W a_1^\dagger \cdots a_{n-1}^\dagger a_n^\dagger | 0 \rangle \geq 0, \quad (21)$$

for all $a_k^\dagger \in \mathcal{B}(\mathcal{F}_1^d)$. Note however that to satisfy Eq.21, it is sufficient that the operator $a_{n-1} \cdots a_1 W a_1^\dagger \cdots a_{n-1}^\dagger$ be positive semidefinite. Thus follows directly that the operator W satisfying the problem in Eq.20 corresponds to an optimal entanglement witness.

The RSDP given above is solved by means of probabilistic relaxations in terms of SDPs, as done in [14], where the set of infinite constraints is exchanged by a finite sample. Thus the witness operator obtained is such that satisfy most of the constraints in Eq.20. The small probability (ϵ) that a constraint be violated (i.e. $Tr(W\sigma) < 0$) diminishes as the size of the sample of constraints increases.

The constraint $\mathcal{A}W\mathcal{A}^\dagger = W$ restricts the operator to the space of antisymmetric entanglement witnesses ($\mathcal{W}(\mathcal{F}_n^d) = \mathcal{A}W\mathcal{A}^\dagger$). The other constraint, $W \leq \mathcal{A}$, follows directly from the anti-symmetrization of Eq.4, and implies that the OEW corresponds to the anti-symmetrized version of the Generalized Robustness, namely,

$$\mathcal{R}_g^{\mathcal{F}}(\rho) = \max(0, - \min_{\mathcal{M}=\{W \in \mathcal{W}(\mathcal{F}_n^d) | W \leq \mathcal{A}\}} Tr(W\rho)). \quad (22)$$

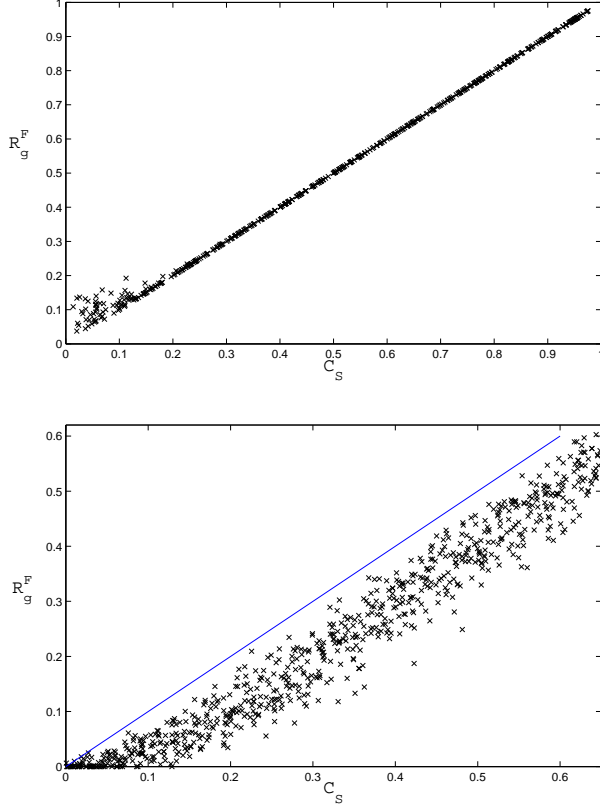


FIG. 1: Fermionic Generalized Robustness $\mathcal{R}_g^{\mathcal{F}}$ versus Schliemann Concurrence C_S , for random fermionic states uniformly distributed according to the Haar measure. (TOP) The two entanglement measures are equal for pure states. The small dispersion seen in the top panel is due to numerical imprecision in the calculation of $\mathcal{R}_g^{\mathcal{F}}$ in the region of very low entanglement. (BOTTOM) In the case of mixed states, the C_S is an upper bound to $\mathcal{R}_g^{\mathcal{F}}$. The continuous line in the bottom panel corresponds to the straight line $C_S = \mathcal{R}_g^{\mathcal{F}}$, and is just a guide to the eye.

$\mathcal{R}_g^{\mathcal{F}}(\rho)$ measures the minimum required mixture with a fermionic state such that all the entanglement of ρ is washed out. In other words, the Generalized Robustness is the minimum value of s such that

$$\sigma = \frac{\rho + s\varphi_f}{1 + s} \quad (23)$$

be a separable state (Eq.17), where φ_f can be any fermionic state.

Fermionic Geometric Discord: Abiding by the notion that mere anti-symmetrization does not generate any kind of quantum correlation, we are led to the following definition of fermionic states without quantum discord:

$$\xi_A = \mathcal{A} \xi \mathcal{A}^\dagger, \quad (24)$$

where \mathcal{A} is the anti-symmetrization operator, and ξ are the states in Eq.15, which encode classical probability

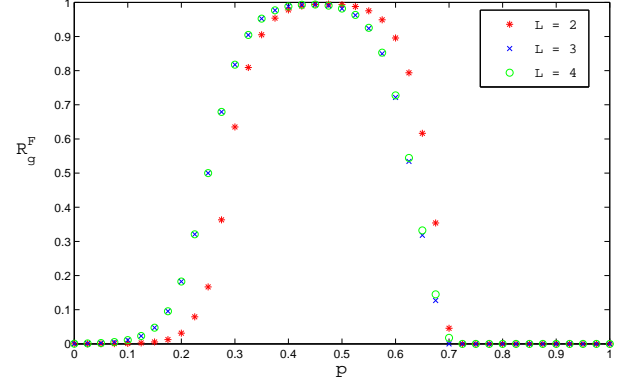


FIG. 2: Fermionic Generalized Robustness $\mathcal{R}_g^{\mathcal{F}}$ for the families of two-fermion states defined in Eq.26, on the space $\mathcal{A}(\mathcal{H}^{(2L)} \otimes \mathcal{H}^{(2L)})$.

distributions. Although these states do not have any kind of quantum correlations, they cannot be treated like classical probability distributions, since they respect quantum rules: like the Pauli exclusion principle.

Our proposed measure for the quantum discord in fermionic states will be a geometric measure like Eq.16. Given a fermionic state $\rho \in \mathcal{A}(\mathcal{H}^{(d)} \otimes \mathcal{H}^{(d)})$, the Fermionic Geometric Discord is given by,

$$\mathcal{D}_f(\rho) = \min_{\xi \in \Omega_A} |\xi - \rho|_1, \quad (25)$$

where $\Omega_A = \mathcal{A} \Omega \mathcal{A}^\dagger$ is the set of zero-discord anti-symmetric states (Eq.24).

IV. NUMERICAL RESULTS

In this section we will illustrate our method. We start by investigating *bipartite entanglement* in the space $\mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$, which has the smallest dimension allowing for quantum correlations in fermionic systems. In this case, we can compare the Fermionic Generalized Robustness ($\mathcal{R}_g^{\mathcal{F}}$ - Eq.22) with the Schliemann concurrence (C_S - Eq.9). Then we investigate the bipartite entanglement in a one-parameter family of states in the space $\mathcal{A}(\mathcal{H}^{(2L)} \otimes \mathcal{H}^{(2L)})$, with L going from 2 to 4. We also compare our Fermionic Geometric Discord (\mathcal{D}_f - Eq.25) with the Fermionic Generalized Robustness for another one-parameter family of states in the space $\mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$. We finish with calculations of *multipartite entanglement* in the Extended Hubbard Model (EHM), where $\mathcal{R}_g^{\mathcal{F}}$ can characterize *quantum phase transitions*.

In Fig.1, we plot the Fermionic Generalized Robustness against the Schliemann concurrence for states generated randomly in the space $\mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$. It is remarkable that C_S and $\mathcal{R}_g^{\mathcal{F}}$ are one and the same for pure states, and C_S is an upper bound for $\mathcal{R}_g^{\mathcal{F}}$ in the case of mixed states. Recall that, in the case of two distinguishable

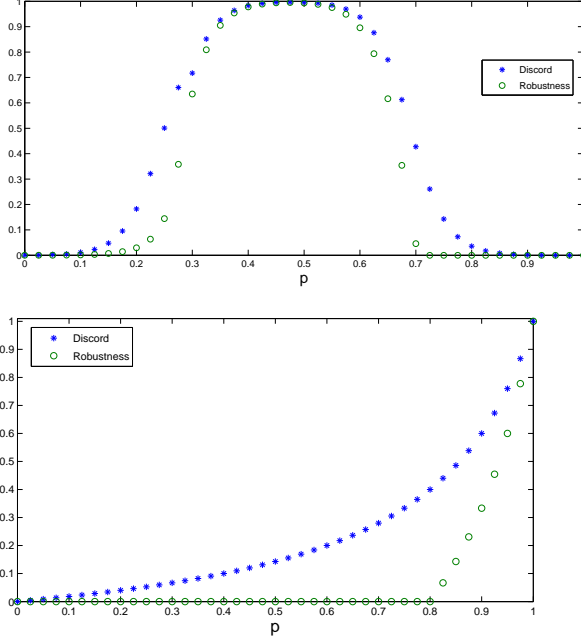


FIG. 3: Fermionic Generalized Robustness $\mathcal{R}_g^{\mathcal{F}}$, and Fermionic Geometric Discord \mathcal{D}_f for the families of two-fermion states defined in Eq.26 (top) and Eq.27 (bottom), on the space $\mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$.

qubits, the Wootters Concurrence [25] and the Generalized Robustness [22] also keep this same relation.

Now we consider the following one-parameter family of states, in the space $\mathcal{A}(\mathcal{H}^{(2L)} \otimes \mathcal{H}^{(2L)})$:

$$\rho = f(0)\sigma + f(1/2)\rho_{max} + f(1)\mathcal{A}, \quad f(x) = Ae^{-\frac{(p-x)^2}{\Delta^2}}, \quad (26)$$

where $\sigma = f_i^\dagger f_j^\dagger |0\rangle$ ($i \neq j$) is a pure state with just a single Slater determinant; ρ_{max} is the maximally entangled pure state of singlet type, i.e. the one with spin quantum numbers $S = S_z = 0$; and \mathcal{A} is the anti-symmetrizer, which corresponds to the identity operator in the antisymmetric space. p controls the entanglement of the state, A is chosen such that the state is normalized, and $\Delta = 0.1826$. In Fig.2, the Fermionic Generalized Robustness is plotted against p , for spaces of different dimensions. We see that $\mathcal{R}_g^{\mathcal{F}}$ behaves correctly, showing that the mixed state has much entanglement when the contribution of the singlet is large, and it has low, or none, entanglement when the contribution of either σ or \mathcal{A} is large.

Consider another one-parameter family of states, in the space $\mathcal{A}(\mathcal{H}^{(4)} \otimes \mathcal{H}^{(4)})$:

$$\rho = (1-p)\mathcal{A} + p\rho_{max}, \quad 0 \leq p \leq 1, \quad (27)$$

In Fig.3, we confront the Fermionic Generalized Robustness and the Fermionic Geometric Discord, for the two families of states (Eq.26, Eq.27) defined above. In the

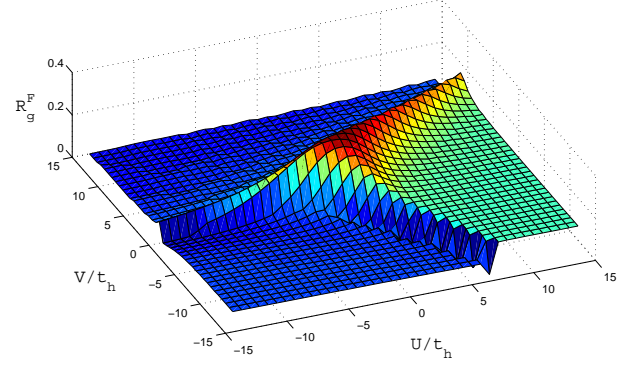


FIG. 4: Five-partite Fermionic Generalized Robustness in the Extended Hubbard Model (Eq.19). The multipartite entanglement works as an order parameter and characterizes quantum phase transitions, in this case, with three distinct phases.

two cases, we see that the discord is always an upper bound for the entanglement, and states without entanglement can have a non-null discord, which is particularly dramatic in the second family. In the first family of states, the functional forms for the discord and entanglement are very similar, whereas they are very different in the second family. Note, in the second family, the abrupt vanishing of entanglement (a discontinuous derivative for $p \cong 0.8$), while the discord shows an asymptotic behavior.

To conclude, we illustrate the calculation of multipartite entanglement of fermions interacting according to the Extended Hubbard Model [21], defined by the Hamiltonian:

$$H_{EHM} = -t_h \sum_{j=1, \sigma=\uparrow, \downarrow}^L (f_{j, \sigma}^\dagger f_{j+1, \sigma} + f_{j+1, \sigma}^\dagger f_{j, \sigma}) + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} + V \sum_{j=1}^L n_j n_{j+1}, \quad (28)$$

where U and V define the on-site and nearest-neighbor Coulomb interactions, t_h controls hopping between sites, L is the number of sites, and $n_{j\sigma}$ is the particle number operator on site j with spin σ . Fig.4 shows the five-partite Fermionic Generalized Robustness of the ground state as a function of U/t_h and V/t_h , for the case of five fermions and five sites. The ground state is obtained by numerical diagonalization of the Hamiltonian. One can see that the Fermionic Generalized Robustness characterizes three distinct regions, corresponding exactly to the three distinct phases provided by the known phase diagram of the model, namely charge-density wave (up), spin-density wave (right) and phase separation (bottom) [21]. It is interesting to note that five fermions in five sites, with periodic boundary conditions, is the smallest size of the system which presents such phase transitions. The occurrence of these phase transitions is dependent on long range interactions. Surprisingly, the second-neighbor interactions present in our five fermions model is already *long range* enough for the onset of phase tran-

sitions. We performed a calculation with four fermions in four sites, and the resulting figure is a uninteresting flat surface for the entanglement.

V. CONCLUSION

In summary, we presented a method to quantify quantum correlations in systems of fermionic indistinguishable particles. The method is based on the use of optimal entanglement witnesses, which can be calculated with arbitrary precision by means of SDPs. In particular, we obtained the Generalized Robustness for fermionic systems ($\mathcal{R}_g^{\mathcal{F}}$), and numerically showed its relation to the Schliemann concurrence. We also introduced the Fermionic Geometric Discord (\mathcal{D}_f), and observed that it is an up-

per bound for the fermionic entanglement. However, the physical meaning of quantum discord for fermionic systems needs to be better understood. It is comforting to know that the quantum discord for a single Slater determinant, or for the fermionic maximally mixed state, is null, but the nature of quantum correlations conveyed by a convex mixture of Slater determinants is still obscure to us, and will be investigated in future works. Finally, we used the five-partite Fermionic Generalized Robustness to characterize quantum phase transitions in the Extended Hubbard Model, showing the utility of entanglement as a quantum order parameter.

Acknowledgments - Financial support by the Brazilian agencies FAPEMIG, CNPq, and INCT-IQ (National Institute of Science and Technology for Quantum Information).

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